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for

Partial Funding of Gordon Research Conference

"Fundamental Interactions of Water with Solid Surfaces"

July 16-20, 1990

Kimball Union Academy

Meriden, NH

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1990 Gordon Research Conference on
 "Fundamental Interactions of Water with Solid Surfaces"

The Gordon Conference on the "Fundamental Interactions of Water with Solid Surfaces" was held from July 16 to 20, 1990 at the Kimball Union Academy in Meriden, NH. The Chairman was Theodore E. Madey of Rutgers University; the Vice-Chairperson was Patricia A. Thiel of Iowa State University. The conference attracted sixty participants; about twenty five percent were from foreign countries, including Canada. There was a good mixture of scientists from universities, national laboratories and private industries, including young scientists and graduate students as well as established scientists.

The program brought together people working in rather different areas, including surface chemistry and physics, electrochemistry, corrosion, wetting, fracture, and processing of semiconductors. The program included eighteen lecturers and nine discussion leaders. The discussion following the talks was unusually active and stimulating, and a large percentage of the attendees contributed to the discussion.

There were a number of exciting new results presented and discussed. P. Norton presented high sensitivity reflection infrared absorption spectroscopic measurements of H_2O on $Ni(110)$, and correlated his results with absolute coverage determinations. Bonzel and White discussed the role of surface additive atoms on the structure and chemistry of H_2C , and demonstrated that a "critical coverage" of adsorbed alkali is necessary for H_2O dissociation to occur. Molecular dynamics simulations of H_2O on metal and oxide surfaces were well covered by Spohr and Garofalini, and their results provided new insights into the structure and reactivity of adsorbed H_2O . Stuve and Wagner described the linkage between surface science and electrochemistry in H_2O -solid interactions, and Wagner reported positive evidence for adsorbed hydronium, H_3O^+ . Chabal described the use of aqueous HF for producing atomically smooth and clean $Si(111)$ surfaces, and Sinclair described the problems caused by moisture in failure of semiconductor electronics.

The role of moisture in fracture of brittle materials was discussed by Lawn, and Porter presented exciting evidence for the structure of H_2O layers between two surfaces at distances of the order 1 nm. Dubois provided the first convincing data showing the relation between surface science (thermal desorption) measurements and macroscopic wetting of surfaces. Finally, Campbell and Kasemo described detailed kinetic schemes for the formation and decomposition of H_2O .

DTC QUALITY REPORT

There were two poster sessions containing a total of twenty four posters of high calibre. All reports I received indicated that the conference was successful and stimulating. The next Gordon Conference on this subject will be scheduled in four to five years, under the chairmanship of Prof. Patricia Thiel, Iowa State University.

Attachments:

1. Conference Program
2. List of Poster Presentations
3. Attendance List

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GORDON RESEARCH CONFERENCE

"Fundamental Interactions of Water With Solid Surfaces" Kimball Union Academy, Meriden, New Hampshire

Theodore E. Madey, Chairman
Rutgers University

Patricia A. Thiel, Vice Chairman
Iowa State University

July 16-20, 1990

Sunday, July 15, 1990

7:00 p.m. Dinner

8:00 p.m. Mixer

Monday, July 16, 1990

8:45 a.m. Introductory Remarks

Morning Session: Water-Metal Interactions

Carsten Benndorf, Discussion Leader

9:00 a.m. Peter Norton
University of Western Ontario

"Interaction of Water with Nickel and
Aluminum Surfaces: Absolute
Coverages, Ordering and Dynamics"

9:50 a.m. Discussion

10:20 a.m. Coffee; Conference Photograph

10:40 a.m. Jose M. Heras
University Nacional de La Plata,
Argentina

"Water on Polycrystalline Metal
Surfaces"

11:30 a.m. Discussion

12:30 p.m. Lunch

Evening Session: Water Interactions With Additives

Galen B. Fisher, Discussion Leader

7:00 p.m. H. P. Bonzel
KFA Julich

"Alkali-Modified Adsorption of
Water"

7:35 p.m. Discussion

8:00 p.m. J. M. White
University of Texas

"Surface Science of Coadsorbate
Overlayers Involving Water"

8:35 p.m. Discussion

Tuesday, July 17, 1990

Morning Session: Theory of H₂O Layers on Surfaces

Uzi Landman, Discussion Leader

- | | | |
|------------|---|---|
| 9:00 a.m. | Eckhard Spohr
University of California | "Computer Simulations of Water on
Metal Surfaces" |
| 9:50 a.m. | Discussion | |
| 10:25 a.m. | Coffee | |
| 10:40 a.m. | J. Woods Halley, Jr.
University of Minnesota | "Electronic Structure and Dynamics at
the Water/Electrode Interface" |
| 11:30 a.m. | Discussion | |
| 12:30 p.m. | Lunch | |

Evening Session: Water at Oxide Surfaces

Richard L. Kurtz, Discussion Leader

- | | | |
|-----------|---|--|
| 7:00 p.m. | Victor E. Henrich
Yale University | "The Interaction of Water with Perfect
and Defect Surfaces of Semiconductors
and Oxides" |
| 7:35 p.m. | Discussion | |
| 7:50 p.m. | Stephen H. Garofalini
Rutgers University | "Water Interactions with Oxide Glass
Surfaces - Molecular Dynamics
Simulations" |
| 8:25 p.m. | Discussion | |
| 8:40 p.m. | Poster Session | |

Wednesday, July 18, 1990

**Morning Session: Electrochemical Aspects of Water-Surface
Interactions**

P. N. Ross, Jr., Discussion Leader

- | | | |
|------------|---|--|
| 9:00 a.m. | Eric Stuve
University of Washington | "In-Situ and Ex-Situ Studies of
Electrochemical Phenomena" |
| 9:50 a.m. | Discussion | |
| 10:25 a.m. | Coffee | |
| 10:40 a.m. | Frederick T. Wagner
General Motors Research Labs | "UHV Investigations of Surface
Solvation Effects in Electrochemistry" |
| 11:30 a.m. | Discussion | |
| 12:30 a.m. | Lunch | |

Evening Session: Interaction of Water With Electronic Materials

Patricia M. George, Discussion Leader

- | | | |
|-----------|--|--|
| 7:00 p.m. | Yves Chabal
AT&T Bell Laboratories | "Infrared Spectroscopy of Water -
Modified Silicon Surfaces" |
| 7:35 p.m. | Discussion | |
| 7:50 p.m. | J. D. Sinclair
AT&T Bell Laboratories | "The Role of Water in the Degradation
of Electronics: Materials, Mechanisms,
Protection, and Challenges" |
| 8:25 p.m. | Discussion | |
| 8:40 p.m. | Poster Session | |

Thursday, July 19, 1990

Morning Session: Interfacial Phenomena

Bruce Bunker, Discussion Leader

- | | | |
|------------|---|---|
| 9:00 a.m. | Brian Lawn
National Institute of Standards
and Technology | "Surface Forces, Adhesion and Fracture
of Brittle Solids" |
| 9:50 a.m. | Discussion | |
| 10:25 a.m. | Coffee | |
| 10:40 a.m. | John D. Porter
Univ. of California, Berkeley | "Interfacial Structure and Dynamics in
Hg/H ₂ O/Hg Tunnel Junction Devices" |
| 11:30 a.m. | Discussion | |
| 12:30 p.m. | Lunch | |

Evening Session: Wetting Phenomena

Mark O. Robbins, Discussion Leader

- | | | |
|-----------|--|--|
| 7:00 p.m. | Michael Schick
University of Washington | "A Theoretical Overview of Wetting
Phenomena" |
| 7:35 p.m. | Discussion | |
| 8:00 p.m. | Lawrence H. Dubois
AT&T Bell Laboratories | "Wetting of Organic Surfaces:
Microscopic Predictions of a
Macroscopic Observable" |
| 8:35 p.m. | Discussion | |

Friday, July 20, 1990

Morning Session: Reactions of H₂O at Surfaces

John T. Yates, Jr., Discussion Leader

8:45 a.m.	Charles T. Campbell University of Washington	"The Water-Gas Shift Reaction Over Clean and Cs-Promoted Cu Single- Crystal Catalysts: Elementary Processes"
9:35 a.m.	Discussion	
10:00 a.m.	Coffee	
10:15 a.m.	Bengt Kasemo Chalmers Univ. of Technology	"Water Formation and Decomposition on Pt"
11:05 a.m.	Discussion	
12:00 noon	Lunch	

Posters Presented at Gordon Conference

"Fundamental Interactions of Water with Solid Surfaces"

Tuesday, July 17, 1990

Dr. G. Pirug
Institut für Grenzflächenforschung
Forschungszentrum Jülich GMBH
Postfach 1913
D-51170 Jülich 1
Federal Republic of Germany

"The Influence of Alkali Metals on the
Oxidation of Si(100) Surfaces by H₂O"
(Authors: G. Pirug and H. P. Bonzel)

Dr. A. Brodsky
Department of Chemistry
University of Pennsylvania
Philadelphia, PA 19104-6323

"Phase Transitions in Surface Water
Layers"

Professor Jiri Skvarla
Department of Mineral Processing
and Environmental Protection
Technical University
Park Komenskeho 19
043 84 Kosice
Czechoslovakia

"A Correlation Between the Wettability
and Aggregation of Fine Minerals"

Robert Brosseau
Department of Chemistry
University of Montreal
Montreal, Quebec, CANADA

"Water on Pd(110)"
(Authors: R. Brosseau and T. H. Ellis)

Brian W. Callen
Department of Chemistry
University of Western Ontario
CANADA N6A 5B7

"Identification of Surface Water
Molecules on Isotopically Substituted
Ice Layers"
(Authors: Brian W. Callen, K. Griffiths
and P. R. Norton)

Professor J. A. Panitz
Department of Physics and
Astronomy
The University of New Mexico
Albuquerque, NM 87131

"Imaging Atom-Probe Studies of Aqueous
Interfaces"

Eric K. Parks
Argonne National Laboratory
701 Lakeside Drive
Hinsdale, IL 60521

"Reactions of Water with Iron, Cobalt,
and Nickel Clusters"
(Authors: E. K. Parks, S. Riley,
T. Klots and B. Winter)

Stephen James Bushby
Department of Chemistry
University of Western Ontario
London, Ontario
CANADA N6A 5B7

"Absolute Hydroxyl Coverage of Oxides
Formed by Water Interaction with
Al(100)"
(Authors: S. J. Bushby, K. Griffiths,
Z. H. Lu, D. K. Greber, R. S. Timsit and
P. R. Norton)

Si-Chung Chang
Department of Chemistry
Purdue University
West Lafayette, IN 47907-3699

"In-Situ Infrared Spectroscopy of Well-
Defined Single Crystal Electrodes"
(Authors: S.-C. Chang and M. Weaver)

Yitzhak Shnidman
Research Laboratories
Eastman Kodak Company
Rochester, NY 14650-2109

"Concentration-Driven Surface Transition
in the Wetting of Mixed Alkanethiol
Monolayers"
(Authors: Y. Shnidman, J. E. Eilers,
S. D. Evans, R. Sharma, J. C. Chang and
A. Ulman)

W.-H. Hung
Department of Chemistry
Princeton University
Princeton, NJ 08544

"The Adsorption of H_2O on Clean and
Oxidized Fe(100)"
(Authors: W.-H. Hung, J. Schwartz and
S. L. Bernasek)

Wednesday, July 18, 1990

Dr. Geoff Thornton
Chemistry Department
Manchester University
Manchester M13 9PL
United Kingdom

" H_2O Adsorption on BSSCO (001) and Other
Oxide Surfaces"

Dr. Rudolf Schubert
Room 3X 215
Bellcore
P. O. Box 7040
Red Bank, NJ 07701-7040

"The Effect of Relative Humidity on
Electrical Contacts"

Dr. Richard Kurtz
Surface Science Division
National Institute for Science
and Technology
Gaithersburg, MD 20899

"The Role of Surface Defects in Water
Chemisorption on $TiO_2(110)$ "

Dr. Ben Ocko
Department of Physics
Brookhaven National Laboratory
Upton, Long Island, NY 11973

"In-Situ X-ray Scattering Investigations
of Electrode Surface Reconstructions"

Dr. Brian Maschhoff
Department of Physics
Laboratory for Surface Modification
Rutgers, The State University of
New Jersey
P. O. Box 849
Piscataway, NJ 08855-90849

"Interaction of Water with Insulator
Surfaces"
(Authors: Brian Maschhoff, J. M. Pan,
M. Szymonski and T. E. Madey)

Dr. D. R. Baer
Surface Physics Group
Battelle Pacific NW Lab
Battelle Blvd.
Richland, WA 99352

"Interactions of H_2O and Mn with the
Cleavage Surface of $CaCO_3$ "
(Authors: D. R. Baer, D. L. Blanchard
and J. M. Zachara)

Prof. Andrej Wieckowski
Department of Chemistry
University of Illinois
Urbana, IL 61801

"Voltammetry and Surface Science of
Rh(100) and Rh(111) Surfaces"

Dr. Masakatsu Watanabe
Department of Chemistry
University of Pennsylvania
Philadelphia, PA 19104-6323

"Phase Transition of Water Between
Metal Surfaces"

Dr. Fred Wagner
Physical Chemical Dept.
General Motors Research Labs
30500 Mound Road
Warren, MI 48090-9055

"Hydrogen and Water Coadsorption on
 $Cu(110)$ and $Pt(111)$: the Formation
of H_3O^+ ?"

Prof. J. Michael White
Department of Chemistry
University of Texas
Austin, Texas 78712

"Optical Absorption of $H_2O(g)$ and
Amorphous Ice"

Dr. Patricia M. George
Aerojet Electro Systems
Surface and Contam. Dept.
P. O. Box 296
Azusa, CA 91702

"The Reaction of Water on $GaAs(100)$ "

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"An XPS Study of Water Removal from
Be at 160K: Evidence for Ion Beam-
Induced Oxidation"

Prof. Doug Doren
Department of Chemistry
University of Delaware
Newark, DE 19716

"Molecular Diffusion on Solid Surfaces:
How Chemisorbed Molecules Differ from
Atoms"

GORDON RESEARCH CONFERENCES

FUNDAMENTAL INTERACTION OF WATER WITH SOLID SURFACES

Kimball Union Academy, Meriden, N.H. 03770

July 16 - 20, 1990

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